Switching mechanism in the $B_{\mathbf{1RevTilted}}$ phase of bent-core liquid crystals

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Abstract

The $B_{1\mathrm{RevTilted}}$ is a uniformly smectic tilted columnar phase in which the macroscopic polarization can be reorientated via electric field. To study the effects on the reorientation mechanism of the various physical parameters, we analyze a local, and a non-local Landau-de Gennes-type energy functional. For the case of large columnar samples, we show that both energies give the same qualitative behavior, with a relevant role played by the terms that describe the interaction between polarization and nematic directors. We also obtain existence of the L^2-gradient flow in metric spaces for the full local energy.

Key words. Bent-core molecules, liquid crystals, columnar phases, Γ-convergence, energy minimization, gradient flow

AMS subject classifications. 76A15, 49J99

1 Introduction

The characteristic banana shape of bent-core molecule liquid crystals (BLCs) allows for spontaneous polar order of the shorter molecular axis, which translates in the possibility of obtaining ferroelectric phases in achiral materials. Achiral ferroelectric liquid crystals are of substantial application interest, which explains the concentration of efforts, seen in recent years, to better understand theoretically and experimentally the many phases of bent-core materials, [12, 2013].

The $B_{1\mathrm{RevTilted}}$ is a columnar phase proper of BLCs in which is possible to reorient the spontaneous polarization by applying an electric field, [17, 2005]. Because of the bow shape of the molecules, the reorientation of the polarization can be

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achieved either by a rotation around the smectic cone or by a rotation around the molecular axis, or by a combination of both. Vaupotič and Čopič in [26, 2005] propose a Landau-de Gennes-type free energy density to study polarization-modulated layer-undulated phases of BLCs. The key feature of their model is the coupling term between the polarization splay, and the tilt of the molecules with the respect to the normal vector of the smectic layers. In [14, 2015], we prove existence of minimizers for the associated energy functional, and study via Γ-convergence a simplified version, considered by Gorecka et al. in [17, 2005] to model experimental results of switching via electric field in the $B_{1\mathrm{RevTilted}}$ phase. Without deriving a closed form for the limiting functional, in [14] we obtain a sufficient condition under which the global minimizers of the limiting functional indicate switching by rotation around the molecular axis, confirming experiments and numerical computations presented in [17]. In here, we improve upon these results, first by finding the explicit expression of the limiting functional, then by using it to infer an estimate that confirms our numerical computations. In particular, while in [17] it is noted that the degree of the tilt, the intensity of the applied electric field and the relative size of the elastic coefficients have a role in determining the type of switching, our analytical and numerical results indicate that switching by rotation around the molecular axis might still not be present, if the magnitude of the coefficient of the term coupling the polarization, the nematic director, and the layer normal is small.

In [17], the authors argue that both Dirichlet and Neumann boundary conditions are of interest, since they correspond to different but relevant physical situations. In this work, we consider Dirichlet boundary conditions. For this choice the coupling term between polarization splay and tilt, whose role is central in [26], integrates to zero. It is then natural to ask if conclusions analogous to the ones we find would still hold for a different model. Very few mathematical papers discuss energy functionals for BCLs, an exception is the non-local energy introduced in [5, 2007] to study BCLs fibers, and rigorously analyzed in [6, 2012]. According to [12, 2013], this energy can be adapted to include the $B_{1\mathrm{RevTilted}}$ phase, and since it also true that a non-local description for the electric self-interactions, as the one used in [6], is in general considered more accurate than a local one, in this work we also analyze the appropriate modification of the energy in [6]. As expected, the non-local term requires some modification in the proofs, but the new limiting functional is only slightly different, and analogous conclusions can be drawn.

The study of the gradient flow of the full local energy, due to the nonlinear constraints, can not be performed in the classical Banach framework, and we need to turn to the more abstract setting provided by the Ambrosio, Gigli and Savaré's theory of gradient flows in metric spaces [2]. Using this approach, we are able to derive in Theorem 6.3 existence of a curve of maximal slope in the weak-L^2 topology.

The paper is organized as follows. In Section 2, we introduce an angular description of the BLCs molecules. In Section 3, we recall the model used in Gorecka et al. [17], and derive a close form for the Γ-limit, using a construction based on classical results contained in [22, 4, 3]. In Section 4, we derive conditions under which the global minimizer of the Γ-limit in Section 3 indicates rotation around the cone, and we present numerical results supporting our claim. In Section 5, we consider the non-local energy in [6], and show that a similar result ensuite. Finally, in Section 6 we prove existence of gradient flow for the full local energy.

2 Background

Bent-core molecules have a peculiar bow-like shape that can be described by two orthogonal unit vectors: the nematic director $\mathbf{n}$ along the direction of the axis of the molecule, and the polarization director $\mathbf{p}$ in the direction of the bow of the molecule, which is the same as the direction of the spontaneous polarization $\mathbf{P} = P\,\mathbf{p}$.

A representation of the two directors and of the layer normal, that contains implicitly the constraints $|\mathbf{n}| = |\mathbf{p}| = 1$ and $\mathbf{n} \cdot \mathbf{p} = 0$, can be given in terms of four angles: the tilt angle θ, the azimuthal angle ϕ, the layer tilt angle Δ, and the polar angle α, [26, 6]. Specifically, we denote by $\boldsymbol{\nu}$ the layer normal, and take the layer tilt angle Δ to be defined modulo 2π as the angle from the z-axis toward the x-axis about the positive y-axis. The tilt angle θ is the angle between $\mathbf{n}$ and $\boldsymbol{\nu}$, that is $\mathbf{n} \cdot \boldsymbol{\nu} = \cos\theta$, and has values $0 \leq \theta \leq \pi$. We define the azimuthal angle $\phi \in [0, 2\pi)$ as the angle from $\boldsymbol{t}$ toward $\boldsymbol{s}$ about $\boldsymbol{\nu}$, where $\boldsymbol{t}$ is the unit vector in the x-z plane perpendicular to $\boldsymbol{\nu}$, and such that $\boldsymbol{t} \times \boldsymbol{\nu}$ is in the negative y direction; while $\boldsymbol{s}$ is a unit vector in the $\boldsymbol{\nu}$-$\mathbf{n}$ plane, perpendicular to $\boldsymbol{\nu}$ and such that $\mathbf{s} \times \boldsymbol{\nu}$ is in the same direction as $\mathbf{n} \times \boldsymbol{\nu}$. Finally, the polar angle α is the angle obtained from $\mathbf{n} \times \boldsymbol{\nu}$ to $\mathbf{p}$ about $\mathbf{n}$, with $\alpha \in (-\pi, \pi]$. Note that α and ϕ are not well-defined if $\mathbf{n}$ and $\boldsymbol{\nu}$ are parallel, therefore this representation needs to be used with care if the tilt angle is allowed to take the values 0 and/or π, unless the tilt is constant. (See Figure 1)

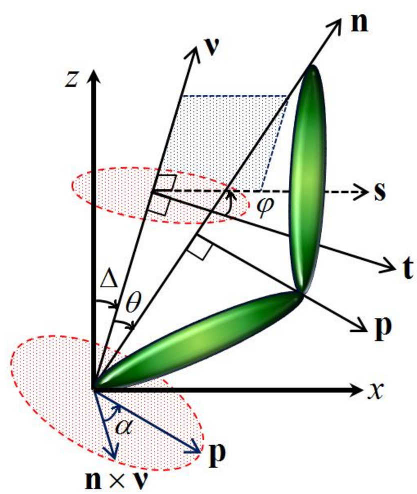

Figure 1: Angular representation of the polar and nematic directors

The angular representation of the layer normal, and directors is given by the equations below:

$$
\begin{aligned}
\boldsymbol{\nu} &=< \sin\Delta, 0, \cos\Delta >;\\
\mathbf{n} &=< \sin\Delta\cos\theta + \sin\theta\cos\phi\cos\Delta,\\
&\qquad \sin\theta\sin\phi,\ \cos\theta\cos\Delta - \sin\theta\sin\Delta\cos\phi >;\\
\mathbf{p} &=< -\sin\alpha\sin\theta\sin\Delta + \sin\alpha\cos\theta\cos\Delta\cos\phi + \sin\phi\cos\Delta\cos\alpha,\\
&\qquad \sin\alpha\cos\theta\sin\phi - \cos\phi\cos\alpha,\\
&\qquad -\sin\alpha\sin\theta\cos\Delta - \sin\alpha\cos\theta\cos\phi\sin\Delta - \sin\phi\sin\Delta\cos\alpha > .
\end{aligned} \tag{1}
$$

3 Local Model

To model experiments exploring the mechanism that guides the reorientation due to an applied electric field of the spontaneous polarization in the $B_{1\mathrm{RevTilted}}$ phase, Gorecka et al., [17], use the free energy density:

$$f(\mathbf{n},\mathbf{p}) = \frac{1}{2}K_n \left[(\nabla\cdot\mathbf{n})^2 + |\nabla\times\mathbf{n}|^2\right] + \frac{1}{2}K_p\left(\nabla\cdot\mathbf{p} - c_0\right)^2 \\ +\frac{1}{2}\,K_{np}\,|\mathbf{p}\times(\mathbf{n}\times\boldsymbol{\nu})|^2 + \frac{P_0^2}{2\bar{\epsilon}\epsilon_0}\,p_1^2 - P_0\,\mathbf{p}\cdot\mathbf{E}. \tag{2}$$

The energy density (2) is built from the one proposed in [26], by adding an interaction term between the polarization and the external field $\mathbf{E}$, and making the following assumptions derived from experimental evidences: the phenomenon is essentially one dimensional in space, the magnitude of the polarization and the tilt angle are constants, that is $\mathbf{P} = P_0\mathbf{p}$ and $\theta = \theta_B \in (0,\pi)$, and the smectic layer normal and density are also constants.

We denote by L the column width, and following Gorecka et al., we rescale length by L, take the applied electric field to be parallel to the columnar axis, that is $\mathbf{E} = E\,\mathbf{e}_2$, and consider a reference frame with the y-axis parallel to the columnar axis, so that $\boldsymbol{\nu} = \mathbf{e}_3 \equiv < 0,0,1 >$. In terms of the angles in (1), we are assuming $\theta = \theta_B$ and $\Delta = 0$, which imply

$$\begin{aligned}
\boldsymbol{\nu} &= < 0,0,1 >;\\
\mathbf{n} &= < \sin\theta_B\cos\phi,\ \sin\theta_B\sin\phi,\ \cos\theta_B >;\\
\mathbf{p} &= < \sin\alpha\cos\theta_B\cos\phi + \sin\phi\cos\alpha,\ \sin\alpha\cos\theta_B\sin\phi - \cos\phi\cos\alpha,\\
&\qquad\quad -\sin\alpha\sin\theta_B > .
\end{aligned}$$

After some calculations, we have the non-dimensionalized energy functional:

$$\frac{2\bar{\epsilon}\epsilon_0}{P_0^2\,L}\int_0^L f(\mathbf{n},\mathbf{p})\,dx = \int_0^1 g(\mathbf{n},\mathbf{p})\,dx,$$

where

$$g(\mathbf{n},\mathbf{p}) = \frac{1}{2}k_n\left[(n_1')^2 + (n_2')^2\right] + \frac{1}{2}k_p\left(p_1' - c_0 L\right)^2 + \frac{1}{2}k_{np}\,p_3^2 + p_1^2 - k_E\,p_2,$$

with

$$k_n = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2\,L^2}K_n; \quad k_p = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2\,L^2}K_p; \quad k_{np} = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2}K_{np}; \quad k_E = \frac{2\bar{\epsilon}\epsilon_0}{P_0}E. \tag{3}$$

We consider boundary conditions, which reflect the alternating behavior of contiguous columns, see [17, 14]:

$$\mathbf{p}(0) = \mathbf{p}(1) = < 0,-1,0 > \ \text{ and }\ \mathbf{n}(0) = \mathbf{n}(1) = < \sin\theta_B, 0, \cos\theta_B > . \tag{4}$$

All the constants in (3) are positive except k_E, which can be positive or negative depending on the direction of the electric field. We assume $k_E > 0$, since we are interested in forcing the spontaneous polarization inside the domain to point in the direction opposite to the one at the boundary.

We expand the term containing p_1', and add the full gradient $\mathbf{p}$. Up to multiplicative and additive constants, we then arrive to the energy functional:

$$\int_0^1 k_p^{1/2}\left[\frac{k_n}{k_p}|\nabla\mathbf{n}|^2+|\nabla\mathbf{p}|^2\right]+\frac{1}{k_p^{1/2}}\left[k_{np}\,p_3^2+2\,p_1^2+2k_E(1-p_2)\right]\,dx, \tag{5}$$

In the numerical experiments, rotation of the molecules around the cone is seen when the elastic coefficients k_p, k_n are comparable in size but small with respect to the coefficient k_{np} of the coupling term, this is equivalent to considering large columnar samples. Therefore, for $\frac{k_n}{k_p}$ fixed, we set $\Omega=(0,1)$ and $\epsilon=k_p^{1/2}$, and consider the energy functional:

$$\mathcal{G}_\epsilon(\mathbf{u})=\int\limits_\Omega\left(\epsilon\,|\nabla\mathbf{u}|^2+\frac{1}{\epsilon}\,W(\mathbf{u})\right)dx, \tag{6}$$

with $\mathbf{u}(x)\in M\;a.e.$ where

$$\begin{aligned} M=\{\mathbf{u}\in\mathbb{R}^5\text{ s.t. }u_1^2+u_2^2&=\frac{k_n}{k_p}\sin^2\theta_B;\\ u_3^2+u_4^2+u_5^2=1;\qquad & u_1\,u_3+u_2\,u_4+\sqrt{\frac{k_n}{k_p}}\cos\theta_B\,u_5=0\}, \end{aligned} \tag{7}$$

and

$$W(\mathbf{u})=2\,u_3^2+k_{np}\,u_5^2+2\,|k_E|\,(1-u_4). \tag{8}$$

One can easily verify, that because of the orthogonality constraint, W is a double-well potential on M, with $Z=\{\mathbf{u}\in M\text{ s.t. }W(\mathbf{u})=0\}$ given by

$$Z=\left\{\mathbf{u}_\pm\equiv\left(\pm\sqrt{\frac{k_n}{k_p}}\,\sin\theta_B,0,0,1,0\right)\right\}. \tag{9}$$

If we define

$$\mathbf{u}_b=\left(\sqrt{\frac{k_n}{k_p}}\,\sin\theta_B,0,0,-1,0\right), \tag{10}$$

we can reframe the problem as the study of the behavior for $\epsilon\to 0$ of the minimizers of the energy functional:

$$\mathcal{F}_\epsilon(\mathbf{u})=\begin{cases}\mathcal{G}_\epsilon(\mathbf{u}) & \mathbf{u}\in H^1(\Omega,M),\quad \mathbf{u}|_{\partial\Omega}=\mathbf{u}_b\\ \infty & \text{otherwise}\end{cases} \tag{11}$$

To derive the limiting behavior of the energy functional $\mathcal{F}_\epsilon$ we employ Γ-convergence. In particular, we refer to Owen et al. [22] to deal with the boundary conditions, and Baldo [4] and Anzellotti et al. [3] to treat the non-linear constraints.

Compactness of $\mathcal{F}_\epsilon$ in L^1 can be proven as in [14]. In particular, we have the following proposition.

Proposition 3.1 (Compactness)**.** *If $\mathcal{F}_{\epsilon_j}(\mathbf{u}_j)$ is bounded, then there exists a subsequence $\mathbf{u}_{j_k}$ such that as $\epsilon_{j_k} \to 0$ it holds $\mathbf{u}_{j_k} \to \mathbf{u}$ in $L^1(\Omega, \mathbb{R}^5)$, where $\mathbf{u}(x) \in Z$ a.e. and $u_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}} \sin\theta_B\})$.*

The results in [3] are in a general manifold set-up, which we can adapt to our case thanks to the next corollary.

Corollary 3.2. *M is a two-dimensional closed, regular submanifold of $\mathbb{R}^5$.*

Proof. The function $F : \mathbb{R}^5 \to \mathbb{R}^3$ defined as

$$F(u_1, u_2, u_3, u_4, u_5) = (u_1^2 + u_2^2 - \frac{k_n}{k_p} \sin^2\theta_B,$$
$$u_3^2 + u_4^2 + u_5^2 - 1, u_1\, u_3 + u_2\, u_4 + \sqrt{\frac{k_n}{k_p}} \cos\theta_B\, u_5),$$

is such that $M = F^{-1}(0, 0, 0)$, and the Jacobian of F:

$$DF = \begin{pmatrix} 2\,u_1 & 2\,u_2 & 0 & 0 & 0 \\ 0 & 0 & 2\,u_3 & 2\,u_4 & 2\,u_5 \\ u_3 & u_4 & u_1 & u_2 & \sqrt{\frac{k_n}{k_p}} \cos\theta_B \end{pmatrix}$$

has rank 2 at every point of M. The claim follows by Corollary 5.9 pg. 80 in [8]. □

As in [4] and [3], an important role is played by the geodesic distance associated with a degenerate Riemannian metric on M that depends on W:

$$d(\mathbf{u}, \mathbf{v}) = \inf\Big\{ \int_0^1 \sqrt{W(\gamma(t))}\, |\gamma'(t)|\, dt : \gamma \in C^1([0, 1], \mathbb{R}^5), \quad (12)$$
$$\gamma(t) \in M, \gamma(0) = \mathbf{u}, \gamma(1) = \mathbf{v} \Big\}.$$

For a fixed $\mathbf{v} \in M$, we let $\Phi_{\mathbf{v}}(\mathbf{u})$ be the function defined for $\mathbf{u}$ of M to be:

$$\Phi_{\mathbf{v}}(\mathbf{u}) = d(\mathbf{u}, \mathbf{v}). \quad (13)$$

Regardless of the choice of $\mathbf{v} \in M$, the function $\Phi_{\mathbf{v}}$ verifies some interesting and useful properties:

Lemma 3.3. *For any fixed $\mathbf{v} \in M$, the function $\Phi_{\mathbf{v}}(\mathbf{u})$ is Lipschitz continuos on M with respect to the Euclidean distance. Additionally, if I is a bounded interval and $\mathbf{u} \in H^1(I, M)$ then the function $w_{\mathbf{v}}(x) = \Phi_{\mathbf{v}}(\mathbf{u}(x))$ is in $H^1(I)$, and*

$$|w'_{\mathbf{v}}(x)| \le W^{1/2}(\mathbf{u}(x))\, |\nabla\mathbf{u}(x)| \text{ for almost any } x \in I.$$

Proof. Thanks to Corollary 3.2, since M is bounded, these properties can be proven just as equation (4.8) and Lemma 4.2 in [3]. □

Given $u \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}} \sin\theta_B\})$, it is well-known, see [16], that u has a finite number of discontinuities, which we will denote by $N(u)$. We also define for a generic function f defined on Ω, scalar or vector valued, its trace on the boundary, as $\widetilde{f}(1) \equiv f^-(1)$ and $\widetilde{f}(0) \equiv f^+(0)$, where

$$f^-(1) = \lim_{\rho \to 0^+} \frac{1}{\rho} \int_{1-\rho}^{1} f(s)\, ds, \quad \text{and} \quad f^+(0) = \lim_{\rho \to 0^+} \frac{1}{\rho} \int_{0}^{0+\rho} f(s)\, ds,$$

if the limits exist. Note that the trace on the boundary for $u \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}} \sin\theta_B\})$ is well-defined, see [16], and also that if $\mathbf{u} \in H^1(\Omega, M)$, with $\mathbf{u}|_{\partial\Omega} = \mathbf{u}_b$, then $\widetilde{\mathbf{u}}(0) = \widetilde{\mathbf{u}}(1) = \mathbf{u}_b$, see Theorem 8.8 in [9].

We will show that the limiting functional is given by the formula:

$$\mathcal{F}_0(\mathbf{u}) = \begin{cases} 2\, N(u_1)\, d(\mathbf{u}_+, \mathbf{u}_-) + 2\, d(\mathbf{u}_b, \widetilde{\mathbf{u}}(0)) + 2\, d(\mathbf{u}_b, \widetilde{\mathbf{u}}(1)) \\ \qquad \text{if } \mathbf{u}(x) \in Z \; a.e. \text{ and } u_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}} \sin\theta_B\}) \\ \infty \qquad \text{otherwise,} \end{cases} \tag{14}$$

where $N(u_1)$ is the number of discontinuities of the first component of $\mathbf{u}$.

For the Γ-convergence study, we use the following characterization [11]:

Theorem 3.4. *Let $(X, \mathcal{T})$ be a topological space, and let F_h a family of functionals parameterized by h. A functional F_0 is the Γ-limit of F_h as $h \to 0$ in $\mathcal{T}$ iff the two following conditions are satisfied:*

(i) *If $u_h \to u_0$ in $\mathcal{T}$, then $\liminf_{h\to 0} F_h(u_h) \geq F_0(u_0)$.*

(ii) *For all $u_0 \in X$, there exists a sequence $u_h \in X$ such that $u_h \to u_0$ in $\mathcal{T}$, and $\lim_{h\to 0} F_h(u_h) = F_0(u_0)$.*

We start by proving the liminf inequality.

Proposition 3.5. *For every sequence $\{\mathbf{u}_j, \epsilon_j\}$ such that $\mathbf{u}_j \to \mathbf{u}_0$ in $L^1(\Omega, \mathbb{R}^5)$ and $\epsilon_j \to 0$ as $j \to \infty$, it holds*

$$\liminf_{j\to\infty} \mathcal{F}_{\epsilon_j}(\mathbf{u}_j) \geq \mathcal{F}_0(\mathbf{u}_0).$$

Proof. If $\liminf_{j\to\infty} \mathcal{F}_{\epsilon_j}(\mathbf{u}_j) = \infty$ then the inequality is trivially true. If not, we can consider a subsequence j_k such that

$$\lim_{j_k\to\infty} \mathcal{F}_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) = \liminf_{j\to\infty} \mathcal{F}_{\epsilon_j}(\mathbf{u}_j) < \infty,$$

and applying Proposition 3.1 to this subsequence we obtain that $\mathbf{u}_0(x) \in Z$ *a.e.* and $(\mathbf{u}_0)_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}} \sin\theta_B\})$. By possibly passing to a further subsequence, we can assume $\{\mathbf{u}_{j_k}\} \subset H^1(\Omega, M)$, and $\mathbf{u}_{j_k} \to \mathbf{u}_0$ also *a.e.*.

Since $(\mathbf{u}_0)_1$ has a finite number of jump discontinuities, we pick δ small enough so that in the intervals $(-\delta, \delta)$ and $(1-\delta, 1+\delta)$ there are none of such discontinuities, and consider the following extension functions defined on $\Omega_\delta = (-\delta, 1+\delta)$:

$$\widehat{\mathbf{u}}_{j_k}(x) = \begin{cases} \mathbf{u}_b & \text{in } (-\delta, 0), \\ \mathbf{u}_{j_k}(x) & \text{in } \Omega, \\ \mathbf{u}_b & \text{in} (1, 1+\delta) \end{cases} \qquad \widehat{\mathbf{u}}_0(x) = \begin{cases} \mathbf{u}_b & \text{in } (-\delta, 0), \\ \mathbf{u}_0(x) & \text{in } \Omega, \\ \mathbf{u}_b & \text{in} (1, 1+\delta) \end{cases}$$

But Ω is a finite interval, hence the compact embedding of $H^1(\Omega)$ in $C(\bar{\Omega}))$ implies that $\widehat{\mathbf{u}}_{j_k} \in H^1(\Omega_\delta, M)$ and converges to $\widehat{\mathbf{u}}_0$ in $L^1(\Omega_\delta, \mathbb{R}^5)$, again by passing to a further subsequence we can also assume convergence a.e.. Finally, $\widehat{\mathbf{u}}_{j_k}$ is constant in $\Omega_\delta \setminus \Omega$, therefore, [15, Lemma 7.7], we see that

$$|\nabla \widehat{\mathbf{u}}_{j_k}(x)| = \begin{cases} 0 & \text{a.e. in } (-\delta, 0), \\ |\nabla \mathbf{u}_{j_k}(x)| & \text{a.e. in } \Omega, \\ 0 & \text{a.e. in} (1, 1+\delta), \end{cases} \tag{15}$$

In what follows we combine arguments in [20, 22, 3], we start by using (15), and Lemma 3.3 for suitable intervals, to derive

$$\begin{aligned} \mathcal{F}_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) &\geq \int_\Omega 2\,|\nabla \mathbf{u}_{j_k}|\; W^{1/2}(\mathbf{u}_{j_k})\,dx = \int_{\Omega_\delta} 2\,|\nabla \widehat{\mathbf{u}}_{j_k}|\; W^{1/2}(\widehat{\mathbf{u}}_{j_k})\,dx \\ &= \int_{-\delta}^{\delta} 2\,|\nabla \widehat{\mathbf{u}}_{j_k}|\; W^{1/2}(\widehat{\mathbf{u}}_{j_k})\,dx + \int_{\delta}^{1-\delta} 2\,|\nabla \mathbf{u}_{j_k}|\; W^{1/2}(\mathbf{u}_{j_k})\,dx \\ &\quad + \int_{1-\delta}^{1+\delta} 2\,|\nabla \widehat{\mathbf{u}}_{j_k}|\; W^{1/2}(\widehat{\mathbf{u}}_{j_k})\,dx \\ &\geq \int_{-\delta}^{\delta} 2\,|(\widehat{w}^{j_k}_{\mathbf{u}_b})'|\,dx + \int_{\delta}^{1-\delta} 2\,|(w^{j_k}_{\mathbf{u}_-})'|\,dx + \int_{1-\delta}^{1-\delta} 2\,|(\widehat{w}^{j_k}_{\mathbf{u}_b})'|\,dx \end{aligned}$$

where $w^{j_k}_{\mathbf{u}_-}(x) := \Phi_{\mathbf{u}_-}(\mathbf{u}_{j_k}(x))$ and $\widehat{w}^{j_k}_{\mathbf{u}_b}(x) := \Phi_{\mathbf{u}_b}(\widehat{\mathbf{u}}_{j_k}(x))$, note that by Lemma 3.3 these are H^1 functions in their domains of definition. From our construction, it follows that $w^{j_k}_{\mathbf{u}_-} \to w^0_{\mathbf{u}_-} := \Phi_{\mathbf{u}_-}(\mathbf{u}_0)$ in $L^1(\Omega, \mathbb{R}^5)$ and $\widehat{w}^{j_k}_{\mathbf{u}_b} \to \widehat{w}^0_{\mathbf{u}_b} := \Phi_{\mathbf{u}_b}(\widehat{\mathbf{u}}_0)$ in $L^1(\Omega_\delta, \mathbb{R}^5)$, and by standard arguments (see for example [16, 1.9 Theorem]), we gather

$$\liminf_{j_k \to \infty} \mathcal{F}_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) \geq \int_{-\delta}^{\delta} 2\,|(\widehat{w}^0_{\mathbf{u}_b})'|\,dx + \int_{\delta}^{1-\delta} 2\,|(w^0_{\mathbf{u}_-})'|\,dx + \int_{1-\delta}^{1-\delta} 2\,|(\widehat{w}^0_{\mathbf{u}_b})'|\,dx.$$

Recalling the definition of δ and using the coarea formula [16], we arrive at

$$\liminf_{j_k \to \infty} \mathcal{F}_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) \geq 2\,d(\mathbf{u}_b, \widetilde{\mathbf{u}}(0)) + 2\,d(\mathbf{u}_+, \mathbf{u}_-)\,\mathcal{H}^0(\partial A^\delta_{\mathbf{u}_-} \cap (\delta, 1-\delta)) + 2\,d(\mathbf{u}_b, \widetilde{\mathbf{u}}(1)),$$

where

$$A^\delta_{\mathbf{u}_-} = \{x \in (\delta, 1-\delta) :\, \mathbf{u}_0(x) = \mathbf{u}_-\}\,, \tag{16}$$

but the value of $\mathcal{H}^0(\partial A^\delta_{\mathbf{u}_-} \cap (\delta, 1-\delta))$ is equal to the number of discontinuities of the first component of $\mathbf{u}_0$ contained in $(\delta, 1-\delta)$, which by definition of δ are the same as the ones in Ω, and the proposition follows. □

Proposition 3.6. *For any $\mathbf{u}_0 \in L^1(\Omega, \mathbb{R}^5)$, there exists a sequence $\{\mathbf{u}_j, \epsilon_j\}$ such that $\mathbf{u}_j \to \mathbf{u}_0$ in $L^1(\Omega, \mathbb{R}^5)$ and $\epsilon_j \to 0$ as $j \to \infty$, for which*

$$\limsup_{j \to \infty} \mathcal{F}_{\epsilon_j}(\mathbf{u}_j) \leq \mathcal{F}_0(\mathbf{u}_0).$$

Proof. As for the previous proposition, the proof combines arguments from [20, 22, 3], in here we will provide only the essential modifications and refer the reader to the cited works for details.

If $\mathcal{F}_0(\mathbf{u}_0) = \infty$ we take $\mathbf{u}_j = \mathbf{u}_0$ and the conclusion follows, if not then $\mathbf{u}_0(x) \in Z\, a.e.$, and $(\mathbf{u}_0)_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n}{k_p}}\,\sin\theta_B\})$, hence as function in $L^1(\Omega, \mathbb{R}^5)$ we have that $\mathbf{u}_0$ has a finite number of jump discontinuity, and as in the previous proposition we can pick $\delta_0 > 0$ small enough so that for any $\delta < \delta_0$ in the intervals $(0, 2\delta)$ and $(1 - 2\delta, 1)$ there are none of such discontinuities.

For a $\delta < \delta_0$ fixed we consider $A^{\delta}_{\mathbf{u}_-}$ as defined in (16), we will prove the theorem for functions $\mathbf{u}_0$ such that $\mathcal{H}^0(\partial A^{\delta}_{\mathbf{u}_-} \cap \partial(\delta, 1-\delta)) = 0$. This is sufficient since, by Lemma 4.3 in [3], for a given $\mathbf{u}_0$, we can consider a sequence of functions $\mathbf{u}^h$ with $\mathbf{u}^h(x) \in Z\, a.e.$, $(\mathbf{u^h})_1 \in BV((\delta, 1-\delta), \{\pm\sqrt{\frac{k_n}{k_p}}\,\sin\theta_B\})$, $\mathcal{H}^0(\partial A^{\delta}_{\mathbf{u^h_-}} \cap \partial(\delta, 1-\delta)) = 0$, and such that $\mathbf{u}^h \to \mathbf{u}_0$ in $L^1((\delta, 1-\delta), \mathbb{R}^5)$ and $\mathcal{H}^0(\partial A^{\delta}_{\mathbf{u^h_-}} \cap (\delta, 1-\delta)) \to \mathcal{H}^0(\partial A^{\delta}_{\mathbf{u}_-} \cap (\delta, 1-\delta))$, which is enough to obtain the result for $\mathbf{u}_0$ using a diagonal argument.

We next assume that there exist geodesics paths $\gamma_l, \gamma_r, \gamma$ of the distance (12), which connect along M the point $\mathbf{u}_b$ to $\widetilde{\mathbf{u}}(0)$, $\mathbf{u}_b$ to $\widetilde{\mathbf{u}}(1)$, and $\widetilde{\mathbf{u}}(0)$ to $\widetilde{\mathbf{u}}(1)$, respectively. If geodesic paths do not exist, one can use sequences of approximating paths and a diagonal argument as suggested in [3]. We then consider a sequence $\{\epsilon_j\} \to 0$ as $j \to \infty$, such that $\epsilon_j^{1/2}\, length\,\gamma_l < \delta$, $\epsilon_j^{1/2}\, length\,\gamma_r < \delta$, and $\epsilon_j^{1/2}\, length\,\gamma < \delta$. Following a classical argument, we consider

$$\psi^l_j(t) = \int_0^t \frac{\epsilon_j\, |(\gamma_l(s))'|}{(\epsilon_j + W(\gamma_l(s)))^{1/2}}\, ds, \qquad \psi^l_j : [0,1] \to \mathbb{R},$$

and its inverse function $\zeta^l_j : [0, \eta^l_j] \to [0,1]$, where $\eta^l_j := \psi^l_j(1)$. Note that $\eta^l_j < \epsilon_j^{1/2}\, length\,\gamma_l < \delta$, and

$$(\zeta^l_j)' = \frac{(\epsilon_j + W(\gamma_l(\zeta^l_j)))^{1/2}}{\epsilon_j\, |(\gamma_l(\zeta^l_j))'|}. \tag{17}$$

We finally define

$$\chi^l_j(t) = \begin{cases} \mathbf{u}_b & \text{if } t < 0, \\ \gamma_l(\zeta^l_j(t)) & \text{if } 0 \le t \le \eta^l_j, \\ \widetilde{\mathbf{u}}(0) & \text{if } t > \eta^l_j. \end{cases}$$

In a similar manner we obtain ζ^r_j and ζ_j, and define χ^r_j and χ_j. For the set $A^{\delta}_{\mathbf{u}_-}$, we consider the distance function

$$\rho_\delta(x) = \begin{cases} -\operatorname{dist}(x, \partial A^{\delta}_{\mathbf{u}_-}) & \text{if } x \in A^{\delta}_{\mathbf{u}_-}, \\ \operatorname{dist}(x, \partial A^{\delta}_{\mathbf{u}_-}) & \text{if } x \notin A^{\delta}_{\mathbf{u}_-}, \end{cases}$$

which by Lemma 4 in [20] is Lipschitz continuous and verifies $|\rho'_\delta| = 1$ a.e.

The elements of the candidate recovering sequence are as follows:

$$\mathbf{u}_j(x) = \begin{cases} \chi^l_j(x) & \text{if } x \in (0, \eta^l_j), \\ \widetilde{\mathbf{u}}(0) & \text{if } x \in [\eta^l_j, \delta), \\ \chi_j(\rho_\delta(x)) & \text{if } x \in [\delta, 1-\delta), \\ \widetilde{\mathbf{u}}(1) & \text{if } x \in [1-\delta, 1-\eta^r_j), \\ \chi^r_j(1-x) & \text{if } x \in [1-\eta^r_j, 1). \end{cases}$$

The above $\mathbf{u}_j$'s are continuos L^1 functions, for which we have, using the area/coarea formula as in [20, (30)], convergence in $L^1(\Omega,\mathbb{R}^5)$ to $\mathbf{u}_0$, and the fact that M is contain in the ball of radius $\sqrt{1+\frac{k_n}{k_p}\,\sin^2\theta_B}$:

$$
\begin{aligned}
\int_\Omega |\mathbf{u}_j(x)-\mathbf{u}_0(x)|\,dx &\le 2\,\eta_j^l\sqrt{1+\frac{k_n}{k_p}\,\sin^2\theta_B}\\
&\quad+\int_\delta^{1-\delta}|\chi_j(\rho_\delta(x))-\chi_0(\rho_\delta(x))|\,dx+2\,\eta_j^r\sqrt{1+\frac{k_n}{k_p}\,\sin^2\theta_B}\\
&\le 2\,\epsilon_j^{1/2}\sqrt{1+\frac{k_n}{k_p}\,\sin^2\theta_B}\,(length\,\gamma_l+length\,\gamma_r)\\
&\quad+\int_\delta^{1-\delta}|\chi_j(\rho_\delta(x))-\chi_0(\rho_\delta(x))|\,|\rho_\delta'(x)|\,dx\\
&\le C\,\epsilon_j^{1/2}+\int_0^{\eta_j}|\chi_j(t)-\chi_0(t)|\,\mathcal{H}^0\left(S_t^\delta\cap(\delta,1-\delta)\right)\,dt\\
&\le C\,\epsilon_j^{1/2}+\int_0^{\eta_j}|\chi_j(t)-\chi_0(t)|\,\mathcal{H}^0\left(S_t^\delta\cap(\delta,1-\delta)\right)\,dt\\
&\le C\,\epsilon_j^{1/2}+\eta_j\,|\mathbf{u}_+-\mathbf{u}_-|\sup_{|t|\le\eta_j}\mathcal{H}^0\left(S_t^\delta\cap(\delta,1-\delta)\right)\\
&\le C\,\epsilon_j^{1/2}+\epsilon_j^{1/2}\,length\,\gamma\,|\mathbf{u}_+-\mathbf{u}_-|\sup_{|t|\le\eta_j}\mathcal{H}^0\left(S_t^\delta\cap(\delta,1-\delta)\right)\\
&\le C\,\epsilon_j^{1/2}\left(1+\sup_{|t|\le C\epsilon_j^{1/2}}\mathcal{H}^0\left(S_t^\delta\cap(\delta,1-\delta)\right)\right)\to 0\ \text{ as } j\to\infty,
\end{aligned}
$$

in the above, C is a constant independent of j, $S_t^\delta=\{x\in\mathbb{R}:\rho_\delta(x)=t\}$, and

$$
\chi_0(t)=\begin{cases}\mathbf{u}_- & \text{if } t\le 0,\\ \mathbf{u}_+ & \text{if } t>0.\end{cases}
$$

Looking at the derivative of the elements of this sequence, by Lemma 4 in [20] and equation (17), we find that

$$
|\mathbf{u}_j'(x)|=\begin{cases}
\epsilon_j^{-1}\,[\epsilon_j+W(\gamma_l(\zeta_j^l(x)))]^{1/2} & \text{if } x\in(0,\eta_j^l),\\
0 & \text{if } x\in[\eta_j^l,\delta),\\
\epsilon_j{}^{-1}\,[\epsilon_j+W(\gamma(\zeta_j(\rho_\delta(x))))]^{1/2} & \text{if } x\in[\delta,1-\delta),\\
0 & \text{if } x\in[1-\delta,1-\eta_j^r),\\
\epsilon_j^{-1}\,[\epsilon_j+W(\gamma_r(\zeta_j^r(1-x)))]^{1/2} & \text{if } x\in[1-\eta_j^r,1).
\end{cases}\tag{18}
$$

We split $|\mathbf{u}_j'(x)|^2$ in $|\mathbf{u}_j'(x)|\,|\mathbf{u}_j'(x)|$ and use (18) for one of the two terms, we also use (17), when $W(\gamma_l(\zeta_j^l))\neq 0$ to rewrite

$$
\frac{1}{\epsilon_j}\,W(\gamma_l(\zeta_j^l))=\epsilon_j\,|(\gamma_l(\zeta_j^l))'|^2\,|(\zeta_j^l)'|^2-1=\epsilon_j\,|\mathbf{u}_j'|\,|(\gamma_l(\zeta_j^l))'|\,|(\zeta_j^l)'|-1,
$$

and similarly for the term involving γ_r, and, recalling that $|\rho_\delta'|=1$ a.e., for the one involving γ, to gather

$$
\begin{aligned}
F_{\epsilon_j}(\mathbf{u}_j) &\leq 2\int_0^{\eta_j^l}[\epsilon_j + W(\gamma_l(\zeta_j^l(x)))]^{1/2}|(\gamma_l(\zeta_j^l(x)))'|\,|(\zeta_j^l(x))'|\,dx \\
&+2\int_\delta^{1-\delta}[\epsilon_j + W(\gamma(\zeta_j(\rho_\delta(x))))]^{1/2}|(\gamma(\zeta_j(\rho_\delta(x))))'|\,|(\zeta_j(\rho_\delta(x)))'||\rho_\delta'(x)|\,dx \\
&+2\int_{1-\eta_j^r}^1[\epsilon_j + W(\gamma_r(\zeta_j^r(1-x)))]^{1/2}|(\gamma_r(\zeta_j^r(1-x)))'|\,|(\zeta_j^r(1-x))'|\,dx \\
&\leq 2\int_0^1[\epsilon_j + W(\gamma_l(t))]^{1/2}|(\gamma_l'(t)|\;dt + 2\int_0^1[\epsilon_j + W(\gamma_r(t))]^{1/2}|(\gamma_r'(t)|\;dt \\
&+2\sup_{|t|\leq\eta_j}\mathcal{H}^0(S_t^\delta\cap(\delta,1-\delta))\int_0^{\eta_j}[\epsilon_j + W(\gamma(\zeta_j(t)))]^{1/2}|(\gamma(\zeta_j(t))'|\,|\zeta_j'(t)|\,dt \\
&\leq 2\int_0^1[\epsilon_j + W(\gamma_l(t))]^{1/2}|(\gamma_l'(t)|\;dt + 2\int_0^1[\epsilon_j + W(\gamma_r(t))]^{1/2}|(\gamma_r'(t)|\;dt \\
&+2\sup_{|t|\leq\eta_j}\mathcal{H}^0(S_t^\delta\cap(\delta,1-\delta))\int_0^1[\epsilon_j + W(\gamma(t))]^{1/2}|\gamma'(t)|\,dt
\end{aligned}
$$

where we used the fact that $\mathbf{u}_+$ and $\mathbf{u}_-$ are zeros of W, and that the derivatives of ζ_j^l, ζ_j and ζ_j^r are nonnegative according to (17). Taking the limsup of the above inequality, Lemma 4 in [20] gives for any $\delta < \delta_0$:

$$
\begin{aligned}
\limsup_{j\to\infty} F_{\epsilon_j}(\mathbf{u}_j) &\leq 2\,d(\mathbf{u}_b,\widetilde{\mathbf{u}}(0)) + 2\,d(\mathbf{u}_b,\widetilde{\mathbf{u}}(1)) \\
&+2\,\mathcal{H}^0(\partial A_{\mathbf{u}_-}^\delta\cap(\delta,1-\delta))\,d(\mathbf{u}_+,\mathbf{u}_-),
\end{aligned}
$$

but by definition of δ_0, if $\delta < \delta_0$ we have that $\mathcal{H}^0(\partial A_{\mathbf{u}_-}^\delta\cap(\delta,1-\delta)) = N((\mathbf{u}_0)_1)$. $\square$

4 Global Minimizers of the Limiting Functional

Looking at the formula for the $\Gamma-$limit $\mathcal{F}_0(\mathbf{u})$, we quickly realize that a global minimizer has no discontinuities in u_1, i. e. $N(u_1) = 0$, thus it is either $\mathbf{u}_+$ or $\mathbf{u}_-$, and it is determined by the relative size of the quantities $d(\mathbf{u}_b,\mathbf{u}_-)$ and $d(\mathbf{u}_b,\mathbf{u}_+)$. In particular, the global minimizer is unique unless $d(\mathbf{u}_b,\mathbf{u}_-) = d(\mathbf{u}_b,\mathbf{u}_+)$.

As pointed out in [14, Remark 2], if the global minimizers is $\mathbf{u}_+$, thinking of $\mathbf{u}_b$ as the value at the boundary, its first component would be continuous across the boundary, hence representing rotation around the axis, vice versa $\mathbf{u}_-$ would imply a discontinuous first component, hence suggesting rotation around the cone.

A numerical approximation done using gradient flow equations of the original model written in terms of the tilt and polar angles, and performed to duplicate the numerics presented in [17], suggests that keeping all the values of the parameters as in [17], but varying k_{np}, rotation around the cone is preferred only if $k_{np} > 2$, see Figure 2, with rotation around the axis favored when $k_{np} \leq 2$, see Figure 3. We note that in [17] all the numerical data provided is for $k_{np} > 2$.

In [14], we show that under some conditions on the other parameters, for k_{np} large enough the global minimizers is indeed $\mathbf{u}_-$, but in our estimates the value of k_{np} for which this happens depends on k_E, that is the larger is k_E the larger k_{np}

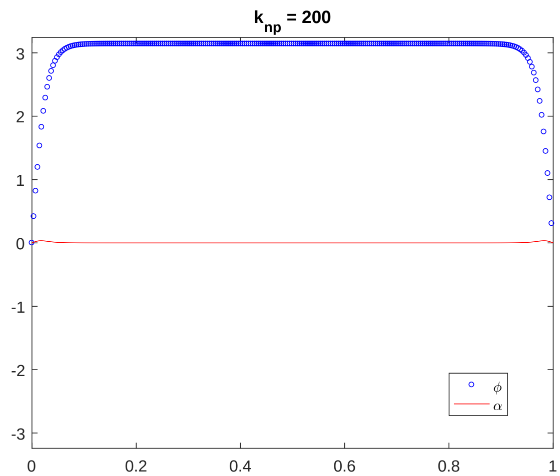

Figure 2: $k_{np} = 200$, $k_n/k_p = 1$

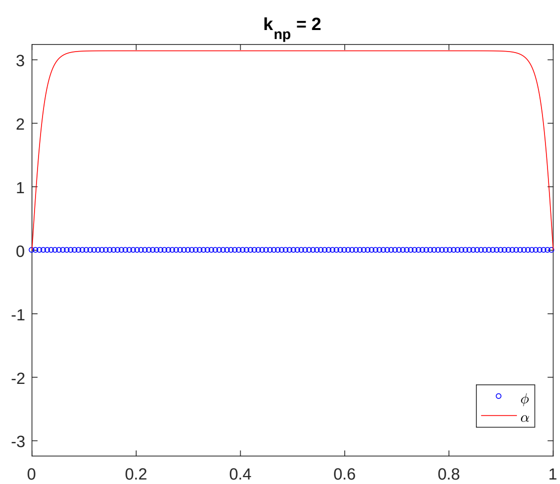

Figure 3: $k_{np} = 2$, $k_n/k_p = 50$

needs to be, a restriction not seen in numerical computations. In fact, our numerical approximations indicate that for the values of the parameters given in [17], for k_E large enough, if $k_{np} > 2$ then $\mathbf{u}_-$ is the global minimizer, while for $k_{np} < 2$ the global minimizer is $\mathbf{u}_+$.

An upper bound for $d(\mathbf{u}_b, \mathbf{u}_+)$ can be found by choosing the test function:

$$\gamma(t) = \left(\sqrt{\frac{k_n}{k_p}}\, \sin\theta_B, 0, \sin\pi t\, \cos\theta_B, -\cos\pi t, -\sin\pi t\, \sin\theta_B \right),$$

namely,

$$d(\mathbf{u}_b, \mathbf{u}_+) \le \int_0^1 \sqrt{(2\cos^2\theta_B + k_{np}\sin^2\theta_B)\sin^2\pi t + 2\,|k_E|\,(1+\cos\pi t)}\;\pi\, dt,$$

which gives

$$\begin{aligned} d(\mathbf{u}_b, \mathbf{u}_+) &\le \sqrt{\max\{2, k_{np}\}} \int_0^1 \sqrt{\sin^2\pi t + |k_E|\,(1+\cos\pi t)}\;\pi\, dt \\ &\le \sqrt{\max\{2, k_{np}\}} \int_0^\pi \sqrt{\sin^2 x + |k_E|\,(1+\cos x)}\, dx \\ &\le \sqrt{\max\{2, k_{np}\}} \int_0^\pi \left(|\sin x| + \sqrt{|k_E|\,(1+\cos x)} \right) dx, \end{aligned}$$

that is

$$d(\mathbf{u}_b, \mathbf{u}_+) \le 2\sqrt{\max\{2, k_{np}\}}\, \left(1 + \sqrt{2}\,\sqrt{|k_E|}\right). \tag{19}$$

It is also possible to find a lower bound for $d(\mathbf{u}_b, \mathbf{u}_-)$, which allows us to obtain the following lemma.

Lemma 4.1. *If $k_{np} < 2$ and $|k_E| \ge 1$, there exists a constant k_{θ_B} depending only on θ_B such that if $\frac{k_n}{k_p} > k_{\theta_B}$ then $\mathbf{u}_+$ is the global minimizer of $\mathcal{F}_0$.*

Proof. We rewrite the potential $W(\mathbf{u})$ as

$$W(\mathbf{u}) = 2\,u_3^2 + k_{np}\,u_5^2 + |k_E|\,\left(A(\mathbf{u}) - \frac{k_p}{k_n}\,\frac{u_1^2}{\sin^2(\theta_B)} \right),$$

where

$$A(\mathbf{u}) = \frac{k_p}{k_n}\,\frac{u_1^2}{\sin^2(\theta_B)} + 2\,(1-u_4),$$

and notice that for $\mathbf{u} \in M$, it holds

$$\inf_{\mathbf{u}\in M} A(\mathbf{u}) = \inf_{\mathbf{v}\in M_0} A_0(\mathbf{v}),$$

where

$$\begin{aligned} M_0 = \{\mathbf{v} \in \mathbb{R}^5 \text{ s.t. } & v_1^2 + v_2^2 = 1; \\ & v_3^2 + v_4^2 + v_5^2 = 1; \qquad v_1\,v_3 + v_2\,v_4 + \cot\theta_B\,v_5 = 0\}, \end{aligned}$$

and

$$A_0(\mathbf{v}) = v_1^2 + 2\,(1-v_4).$$

Hence, $\inf_{\mathbf{u}\in M} A(\mathbf{u})$ depends only on θ_B, also by continuity of A_0 and compactness of M_0 the infimum is attained, that is $L(\theta_B) := \inf_{\mathbf{v}\in M_0} A_0(\mathbf{v}) = A_0(\mathbf{v}_0) \geq 0$. It's easy to see that $L(\theta_B) \leq 1$ (in fact, a direct computation gives strictly less than one), but more importantly $L(\theta_B) > 0$. This can be seen by noticing that $A_0(\mathbf{u}) \neq 0$ for any $\mathbf{v} \in M_0$, as $A_0(\mathbf{v}) = 0$ implies $v_1 = 0$ and $v_4 = 1$. But, $v_4 = 1$ implies $v_3 = v_5 = 0$, and $v_1 = 0$ gives $v_2 = 1$, thus $v_1\, v_3 + v_2\, v_4 + \cot\theta_B\, v_5 = 1 \neq 0$.

In conclusion, we have that

$$0 < \inf_{\mathbf{u}\in M} A(\mathbf{u}) = L(\theta_B) < 1.$$

If we now consider a path $\gamma \in C^1([0,1],\mathbb{R}^5)$, with $\gamma(t) \in M, \gamma(0) = \mathbf{u}_b$, and $\gamma(1) = \mathbf{u}_-$, we have that

$$\begin{aligned}
&\int_0^1 \sqrt{W(\gamma(t))}\,|\gamma'(t)|\,dt \geq \int_0^1 \sqrt{W(\gamma(t))}\left(\frac{|\gamma_1'(t)|}{\sqrt{2}} + \frac{|\gamma_4'(t)|}{\sqrt{2}}\right) dt \\
&\geq \frac{\sqrt{|k_E|}}{\sqrt{2}} \int_{\left\{t\,:\,\gamma_1^2(t) \leq L(\theta_B)\,\frac{k_n}{k_p}\sin^2\theta_B\right\}} \sqrt{L(\theta_B) - \frac{k_p}{k_n}\frac{\gamma_1^2(t)}{\sin^2(\theta_B)}}\,|\gamma_1'(t)|\,dt \\
&\qquad + \frac{1}{\sqrt{2}}\int_0^1 \sqrt{2\,|k_E|\,(1-\gamma_4(t))}\,|\gamma_4'(t)|\,dt \\
&\geq \frac{\sqrt{|k_E|}}{\sqrt{2}}\sqrt{\frac{k_n}{k_p}}\sin\theta_B \int_{-\sqrt{L(\theta_B)}}^{\sqrt{L(\theta_B)}} \sqrt{L(\theta_B) - s^2}\,ds + \int_{-1}^1 \sqrt{|k_E|\,(1-s)}\,ds \\
&= \sqrt{|k_E|}\left(\frac{\pi}{2\sqrt{2}}\sqrt{\frac{k_n}{k_p}}\sin\theta_B\, L(\theta_B) + \frac{4}{3}\sqrt{2}\right).
\end{aligned}$$

In the above, we use the fact that $\gamma_1(t)$ and $\gamma_4(t)$ are continuous functions on $[0,1]$, with $\gamma_1(0) = \sqrt{\frac{k_n}{k_p}}\sin\theta_B$, $\gamma_4(0) = -1$, and $\gamma_1(1) = -\sqrt{\frac{k_n}{k_p}}\sin\theta_B$, $\gamma_4(1) = 1$.

We then can claim that

$$d(\mathbf{u}_b, \mathbf{u}_-) \geq \sqrt{|k_E|}\left(\frac{C(\theta_B)}{\sqrt{2}}\sqrt{\frac{k_n}{k_p}}\sin\theta_B + \frac{4}{3}\sqrt{2}\right),$$

and from this equation (19) implies the lemma. □

5 Non-Local Model

Following the classification presented in [12], the model proposed by Vaupotič and Čopič [26] deals with a material which in the bulk prefers a SmCP phase, while the one in Bauman and Phillips [6] assumes a SmCLP ground state (also known as $\mathrm{SmC_G}$). In a SmCLP structure both the molecular plane and the nematic director are tilted with respect to the layer normal, with fix tilt θ_0 and polar α_0 angles. On the other hand, again according to [12], a SmCP structure can be also described by a double-tilt with fix angle θ_0 and polar angle α_0 equal to either 0 or π.

In our situation, using the definition of α proposed in the previous sections, the ground state has fixed $0 < \theta_0 = \theta_B < \frac{\pi}{2}$ and $\alpha = \pi$, and since (2) is a suitable modified version of the energy density proposed in[26], it seems reasonable to explore if an analogous adaptation of the model in [6], (see also [5, 2007] and [7, 2015]) in the case $\theta_0 = \theta_B, \alpha_0 = \pi$ would lead to similar conclusions.

If we add the interaction term between polarization and external field adopted in (2), assuming constant smectic density and with $\nabla\omega$ denoting the smectic layer normal, we have that the energy density in [6] reads

$$\frac{1}{2}K|\nabla\mathbf{n}|^2 + \frac{1}{2}v|\nabla\mathbf{p}|^2 + \frac{1}{2}\,jq^8\left((\nabla\omega \times \mathbf{n}\cdot\mathbf{p})^2\,(\nabla\omega\cdot\mathbf{n})^2 - \chi_0^2\,|\nabla\omega|^4\right)^2$$
$$+c_p\nabla\cdot\mathbf{p} - P_0\,\mathbf{p}\cdot\mathbf{E} + \frac{\epsilon_0\,\bar{\epsilon}}{2}\,|\nabla\phi|^2 + P_0\,\mathbf{p}\cdot\nabla\phi,$$

with $v, j > 0$, $\chi_0^2 = \sin^2\theta_0\,\cos^2\theta_0\,\cos^2\alpha_0$, $c_p = c' + c''\,P_0 > 0$, and

$$\begin{cases}\epsilon_0\,\bar{\epsilon}\,\nabla\cdot\nabla\phi = P_0\,\nabla\cdot\mathbf{p} & \text{inside sample,}\\ \phi = 0 & \text{on boundary of sample.}\end{cases}$$

Hence, under the same assumptions stated in section 3, the energy becomes:

$$\int_0^L \Big(\frac{1}{2}K|\nabla\mathbf{n}|^2 + \frac{1}{2}v|\nabla\mathbf{p}|^2 + \frac{1}{2}\,jq^8\left((\mathbf{e}_3\times\mathbf{n}\cdot\mathbf{p})^2\,(\mathbf{e}_3\cdot\mathbf{n})^2 - \chi_0^2\right)^2$$
$$+c_p\,p_1' - P_0\,E\,p_2 + \frac{3}{2}\epsilon_0\,\bar{\epsilon}\,|\phi'|^2\Big)\,dx,$$

where $\chi_0^2 = \sin^2\theta_B\,\cos^2\theta_B$, and

$$\begin{cases}\epsilon_0\,\bar{\epsilon}\,\phi'' = P_0\,p_1' & \text{in } [0,L],\\ \phi(0) = \phi(L) = 0\end{cases} \tag{20}$$

The last term in the energy is a non-local term representing the electric self-interactions, which in (2) are approximated by the local simpler term $\dfrac{P_0^2}{2\epsilon\epsilon_0}\,p_1^2$.

Using the fact that under our hypotheses $n_1^2 + n_2^2 = \sin^2\theta_B$, $n_3^2 = \cos^2\theta_B$, $|\mathbf{p}| = 1$, and $\mathbf{n}\cdot\mathbf{p} = 0$, we obtain

$$\begin{aligned}&\left((\mathbf{e}_3\times\mathbf{n}\cdot\mathbf{p})^2\,(\mathbf{e}_3\cdot\mathbf{n})^2 - \chi_0^2\right)^2 = ((n_1p_2 - n_2p_1)^2 n_3^2 - \sin^2\theta_B\,\cos^2\theta_B)^2\\ &= \cos^4\theta_B\,(n_1^2p_2^2 + n_2^2p_1^2 - 2n_1p_2n_2p_1 - \sin^2\theta_B)^2\\ &= \cos^4\theta_B\,(n_1^2 - n_1^2p_1^2 - n_1^2p_3^2 + n_2^2 - n_2^2p_2^2 - n_2^2p_3^2 - 2n_1p_2n_2p_1 - \sin^2\theta_B)^2\\ &= \cos^4\theta_B\,(\sin^2\theta_B - (n_1p_1 + n_2p_2)^2 - \sin^2\theta_B\,p_3^2 - \sin^2\theta_B)^2\\ &= \cos^4\theta_B\,(-n_3^2\,p_3^2 - \sin^2\theta_B\,p_3^2)^2 = \cos^4\theta_B\,(-\cos^2\theta_B\,p_3^2 - \sin^2\theta_B\,p_3^2)^2,\end{aligned}$$

that is

$$(\mathbf{e}_3\times\mathbf{n}\cdot\mathbf{p})^2\,(\mathbf{e}_3\cdot\mathbf{n})^2 = \cos^4\theta_B\,p_3^4.$$

A combination of (20), and the boundary conditions (4), allow us to simplify further the electric self-interaction term:

$$\epsilon_0\,\bar{\epsilon}\,\phi'(x) = P_0\,p_1(x) - P_0\,\frac{1}{L}\int_0^L p_1(x)\,dx.$$

We next non-dimensionalize length by L and multiply by the factor $\dfrac{2\bar{\epsilon}\epsilon_0}{P_0^2\,L}$, to arrive at the functional:

$$\int_0^1 \left(\frac{1}{2} k_n^* |\nabla \mathbf{n}|^2 + \frac{1}{2} k_p^* |\nabla \mathbf{p}|^2 + \frac{1}{2}\, k_{np}^*\, p_3^4 - k_E\, p_2 + 3 \left(p_1 - \int_0^1 p_1\, ds \right)^2 \right) dx,$$

with

$$k_n^* = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2\, L^2} K; \quad k_p^* = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2\, L^2} v; \quad k_{np}^* = \frac{2\bar{\epsilon}\epsilon_0}{P_0^2}\, j q^8 \cos^4\theta_B; \quad k_E = \frac{2\bar{\epsilon}\epsilon_0}{P_0} E. \tag{21}$$

Finally, using the elementary fact that

$$\int_0^1 \left(p_1 - \int_0^1 p_1\, ds \right)^2 dx = \int_0^1 \left(p_1^2 - \left(\int_0^1 p_1\, ds \right)^2 \right) dx, \tag{22}$$

again denoting $\Omega = [0,1]$, and proceeding as in Section 3, we are led to the energy functional

$$\mathcal{G}_\epsilon^*(\mathbf{u}) = \int\limits_\Omega \left(\epsilon\, |\nabla \mathbf{u}|^2 + \frac{1}{\epsilon}\, W^*(\mathbf{u}) - \frac{6}{\epsilon} \left(\int_\Omega u_3\, ds \right)^2 \right) dx, \tag{23}$$

with $\mathbf{u}(x) \in M^*$ *a.e.* where

$$M^* = \{ \mathbf{u} \in \mathbb{R}^5 \text{ s.t. } u_1^2 + u_2^2 = \frac{k_n^*}{k_p^*} \sin^2\theta_B;$$
$$u_3^2 + u_4^2 + u_5^2 = 1; \qquad u_1\, u_3 + u_2\, u_4 + \sqrt{\frac{k_n^*}{k_p^*}} \cos\theta_B\, u_5 = 0 \}, \tag{24}$$

and

$$W^*(\mathbf{u}) = 6\, u_3^2 + k_{np}^*\, u_5^4 + 2\, |k_E|\, (1 - u_4). \tag{25}$$

W^* is a double-well potential on M^*, with set of zeros given by

$$Z^* = \left\{ \mathbf{u}_\pm^* \equiv \left(\pm \sqrt{\frac{k_n^*}{k_p^*}} \sin\theta_B, 0, 0, 1, 0 \right) \right\}. \tag{26}$$

Letting

$$\mathbf{u}_b^* = \left(\sqrt{\frac{k_n^*}{k_p^*}} \sin\theta_B, 0, 0, -1, 0 \right) \tag{27}$$

we are now looking at the behavior for $\epsilon \to 0$ of the minimizers of the energy functional:

$$\mathcal{F}_\epsilon^*(\mathbf{u}) = \begin{cases} \mathcal{G}_\epsilon^*(\mathbf{u}) & \mathbf{u} \in H^1(\Omega, M), \quad \mathbf{u}|_{\partial\Omega} = \mathbf{u}_b^* \\ \infty & \text{otherwise} \end{cases} \tag{28}$$

Thanks to (22), and the following simple inequality, which holds for $\mathbf{u} \in M^*$:

$$\int_0^1 u_3^2\,dx = \int_0^1 \left(1 - u_4^2 - u_5^2\right)\,dx \le 2\int_0^1 (1 - u_4)\,dx,$$

we still have a compactness result:

Proposition 5.1 (Compactness)**.** *If $\mathcal{F}^*_{\epsilon_j}(\mathbf{u}_j)$ is bounded, then there exists a subsequence $\mathbf{u}_{j_k}$ such that as $\epsilon_{j_k} \to 0$ it holds $\mathbf{u}_{j_k} \to \mathbf{u}$ in $L^1(\Omega, \mathbb{R}^5)$ where $\mathbf{u}(x) \in Z^*$ a.e. and $u_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n^*}{k_p^*}}\,\sin\theta_B\})$.*

We believe that the behavior of the functional (23) is qualitatively the same as the one of (2), in particular we would like to show that its limiting functional is given by

$$\mathcal{F}^*_0(\mathbf{u}) = \begin{cases} 2\,N(u_1)\,d^*(\mathbf{u}_+, \mathbf{u}_-) + 2\,d^*(\mathbf{u}_b, \widetilde{\mathbf{u}}(0)) + 2\,d^*(\mathbf{u}_b, \widetilde{\mathbf{u}}(1)) \\ \qquad\qquad \text{if } \mathbf{u}(x) \in Z^* \text{ a.e. and } u_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n^*}{k_p^*}}\,\sin\theta_B\}) \\ \infty \qquad\qquad \text{otherwise,} \end{cases} \tag{29}$$

where $N(u_1)$ is the number of discontinuities of the first component of $\mathbf{u}$, and

$$d^*(\mathbf{u}, \mathbf{v}) = \inf\Big\{ \int_0^1 \sqrt{W^*(\gamma(t))}\,|\gamma'(t)|\,dt : \gamma \in C^1([0,1], \mathbb{R}^5), \\ \gamma(t) \in M^*, \gamma(0) = \mathbf{u}, \gamma(1) = \mathbf{v}\Big\}, \tag{30}$$

which as before is a geodesic distance associated with a degenerate Riemann metric on a manifold M^* that depends on W^*.

An analogous of Proposition 3.6 can be proven in exactly the same way, since in here we are subtracting from a double-well potential the positive term $\dfrac{6}{\epsilon}\left(\displaystyle\int_\Omega u_3\,ds\right)^2$:

Proposition 5.2. *For any $\mathbf{u}_0 \in L^1(\Omega, \mathbb{R}^5)$, there exists a sequence $\{\mathbf{u}_j, \epsilon_j\}$ such that $\mathbf{u}_j \to \mathbf{u}_0$ in $L^1(\Omega, \mathbb{R}^5)$ and $\epsilon_j \to 0$ as $j \to \infty$, for which*

$$\limsup_{j\to\infty} \mathcal{F}^*_{\epsilon_j}(\mathbf{u}_j) \le \mathcal{F}^*_0(\mathbf{u}_0).$$

It's instead less clear, if it's possible to derive an analogous of Proposition 3.5.

Given a sequence $\{c(\epsilon)\}$, such that $c(\epsilon) \to 0$ as $\epsilon \to 0$, for $\mathbf{u} \in M^*$ we consider

$$W^*_\epsilon(\mathbf{u}) = 6\,(u_3 - c(\epsilon))^2 + k^*_{np}\,u_5^4 + 2\,|k_E|\,(1 - u_4), \tag{31}$$

and introduce

$$d^*_\epsilon(\mathbf{u}, \mathbf{v}) = \inf\Big\{ \int_0^1 \sqrt{W^*_\epsilon(\gamma(t))}\,|\gamma'(t)|\,dt : \gamma \in C^1([0,1], \mathbb{R}^5), \\ \gamma(t) \in M^*, \gamma(0) = \mathbf{u}, \gamma(1) = \mathbf{v}\Big\}. \tag{32}$$

Remark 1. Following [3, pg 183-185], since W^*_ϵ is never zero in M^* when $c(\epsilon) \neq 0$, while if $c(\epsilon) = 0$ then $d^*_\epsilon \equiv d^*$, using the fact that for ϵ small enough, it holds $\sup_{M^*} \sqrt{W^*_\epsilon} < C^*$ with C^* independent of ϵ, we have the following properties:

(1) d^*_ϵ is a metric on M^*;

(2) $d^*_\epsilon(\mathbf{u}, \mathbf{v}) \to d^*(\mathbf{u}, \mathbf{v})$ as $\epsilon \to 0$;

(3) For $\mathbf{v} \in M^*$ fixed, if $\mathbf{u}_\epsilon \to \mathbf{u}$ as $\epsilon \to 0$, then $d^*_\epsilon(\mathbf{u}_\epsilon, \mathbf{v}) \to d^*(\mathbf{u}, \mathbf{v})$, since (see [3, (4.9) & (4.10)])

$$\begin{aligned}&|d^*_\epsilon(\mathbf{u}_\epsilon, \mathbf{v}) - d^*(\mathbf{u}, \mathbf{v})| \leq |d^*_\epsilon(\mathbf{u}_\epsilon, \mathbf{v}) - d^*_\epsilon(\mathbf{u}, \mathbf{v})| + |d^*_\epsilon(\mathbf{u}, \mathbf{v}) - d^*(\mathbf{u}, \mathbf{v})| \\ &\leq |d^*_\epsilon(\mathbf{u}_\epsilon, \mathbf{u})| + |d^*_\epsilon(\mathbf{u}, \mathbf{v}) - d^*(\mathbf{u}, \mathbf{v})| \leq C_1 C^* |\mathbf{u}_\epsilon - \mathbf{u}| + |d^*_\epsilon(\mathbf{u}, \mathbf{v}) - d^*(\mathbf{u}, \mathbf{v})|;\end{aligned}$$

(4) If we define

$$\Phi^*_{\mathbf{v}}(\mathbf{u}) = d^*(\mathbf{u}, \mathbf{v}) \quad \text{and} \quad \Phi^*_{\epsilon,\mathbf{v}}(\mathbf{u}) = d^*_\epsilon(\mathbf{u}, \mathbf{v}), \tag{33}$$

the analogous of Lemma 3.3 holds for both $\Phi^*_{\mathbf{v}}$ and $\Phi^*_{\epsilon,\mathbf{v}}$ with M^*, and

$$w^*_{\mathbf{v}}(x) = \Phi^*_{\mathbf{v}}(\mathbf{u}(x)) \quad \text{and} \quad w^*_{\epsilon,\mathbf{v}}(x) = \Phi^*_{\epsilon,\mathbf{v}}(\mathbf{u}(x)); \tag{34}$$

(5) For $\mathbf{v} \in M^*$ fixed and $\mathbf{u}_\epsilon \in L^1(\Omega, M^*)$, if $\mathbf{u}_\epsilon(x) \to \mathbf{u}(x)$ a.e. as $\epsilon \to 0$, and

$$w^{*;\epsilon}_{\epsilon,\mathbf{v}}(x) := \Phi^*_{\epsilon,\mathbf{v}}(\mathbf{u}_\epsilon(x)),$$

then

$$w^{*;\epsilon}_{\epsilon,\mathbf{v}}(x) \to w^*_{\mathbf{v}}(x) \quad \text{a.e.},$$

as can be seen by applying (1) and (2) above, since

$$\begin{aligned}&|w^{*;\epsilon}_{\epsilon,\mathbf{v}}(x) - w^*_{\mathbf{v}}(x)| \\ &\quad\leq |d^*_\epsilon(\mathbf{u}_\epsilon(x), \mathbf{v}) - d^*_\epsilon(\mathbf{u}(x), \mathbf{v})| + |d^*_\epsilon(\mathbf{u}(x), \mathbf{v}) - d^*(\mathbf{u}(x), \mathbf{v})|;\end{aligned}$$

(6) Let $O \subset \mathbb{R}$ be an open bounded set. For $\mathbf{v} \in M^*$ fixed, if $\mathbf{u}_\epsilon \subset H^1(O, M^*)$, and $\mathbf{u}_\epsilon \to \mathbf{u}$ in $L^1(O, \mathbb{R}^5)$ and *a.e.*, with $\mathbf{u}(x) \in Z^*$ *a.e.* and $u_1 \in BV(\Omega, \{\pm\sqrt{\frac{k^*_n}{k^*_p}}\, \sin\theta_B\})$, then

$$w^{*;\epsilon}_{\epsilon,\mathbf{v}} \to w^*_{\mathbf{v}} \quad \text{in } L^1(O),$$

and by [16, 1.9 Theorem]

$$\liminf_{\epsilon\to 0} \int_O |(w^{*;\epsilon}_{\epsilon,\mathbf{v}})'|\, dx \geq \int_O |(w^*_{\mathbf{v}})'|\, dx.$$

Convergence of $w^{*;\epsilon}_{\epsilon,\mathbf{v}}$ to $w^*_{\mathbf{v}}$ in $L^1(O)$ is a consequence of (5), O bounded, M^* contained in the ball of radius $\sqrt{1 + \frac{k^*_n}{k^*_p} \sin^2\theta_B}$, and the fact that under our assumptions for ϵ small enough, we have

$$|(w^{*;\epsilon}_{\epsilon,\mathbf{v}})(x)| \leq C_1\, C^*\, |\mathbf{u}_\epsilon(x) - \mathbf{v}| \leq 2\, C_1\, C^* \sqrt{1 + \frac{k^*_n}{k^*_p} \sin^2\theta_B},$$

so that we can apply the Lebesgue dominated convergence theorem.

Proposition 5.3. *For every sequence $\{\mathbf{u}_j, \epsilon_j\}$ such that $\mathbf{u}_j \to \mathbf{u}_0$ in $L^1(\Omega, \mathbb{R}^5)$ and $\epsilon_j \to 0$ as $j \to \infty$, it holds*

$$\liminf_{j\to\infty} \mathcal{F}^*_{\epsilon_j}(\mathbf{u}_j) \geq \mathcal{F}^*_0(\mathbf{u}_0).$$

Proof. If $\liminf_{j\to\infty} \mathcal{F}^*_{\epsilon_j}(\mathbf{u}_j) = \infty$ then the inequality is true. If not, we can consider a subsequence j_k such that

$$\lim_{j_k\to\infty} \mathcal{F}^*_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) = \liminf_{j\to\infty} \mathcal{F}^*_{\epsilon_j}(\mathbf{u}_j) < \infty,$$

and applying Proposition 5.1 to this subsequence we obtain that $\mathbf{u}_0(x) \in Z^*$ *a.e.* and $(\mathbf{u}_0)_1 \in BV(\Omega, \{\pm\sqrt{\frac{k_n^*}{k_p^*}}\sin\theta_B\})$. By possibly passing to a further subsequence, we can assume $\{\mathbf{u}_{j_k}\} \subset H^1(\Omega, M^*)$, and $\mathbf{u}_{j_k} \to \mathbf{u}_0$ also *a.e.*.

On the other hand, $\mathbf{u}_0(x) \in Z^*$ *a.e.* implies $(\mathbf{u}_0)_3(x) = 0$ *a.e.*, and by L^1 convergence we have

$$c(\epsilon_{j_k}) := \int_\Omega (\mathbf{u}_{j_k})_3 \, dx \to 0. \tag{35}$$

Noticing that the elements of this subsequence verify

$$\mathcal{F}^*_{\epsilon_{j_k}}(\mathbf{u}_{j_k}) = \int_\Omega \left(\epsilon\,|\nabla\mathbf{u}|^2 + \frac{1}{\epsilon}\,W^*_{\epsilon_{j_k}}(\mathbf{u})\right) dx,$$

we conclude that thanks to Remark 1, the theorem follows as in the proof of Proposition 3.5. □

6 Gradient Flow

To conclude our study, we address the question of existence of the gradient flow relative to the local energy (5). In what follows, to simplify notations and without loss of generality, we set all the physical constants to be equal to one.

We define the functional space

$$\mathcal{M} := \{(\mathbf{p},\mathbf{n}) \in W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3) : |\mathbf{p}| = |\mathbf{n}| = 1,\ n_3 = \cos\theta_B,\ \mathbf{p}\cdot\mathbf{n} = 0\},$$

and study the gradient flow for the energy, $G : \mathcal{M} \longrightarrow \mathbb{R}$,

$$G(\mathbf{p},\mathbf{n}) := \int_\Omega \left[|\nabla\mathbf{p}|^2 + |\nabla\mathbf{n}|^2 + \mathcal{W}(\mathbf{p})\right] dx,$$

subject to the boundary conditions (4), with $\Omega = [0,1]$, and

$$\mathcal{W}(\mathbf{p}) = 2\,p_1^2 + p_3^2 + 2\,(1 - p_2).$$

Since the set

$$V := \{(\mathbf{p},\mathbf{n}) \in \mathcal{M} : \mathbf{p}(0) = \mathbf{p}(1) = (0,-1,0), \mathbf{n}(0) = \mathbf{n}(1) = (\sin\theta_B, 0, \cos\theta_B)\}$$

is not a Banach space with respect to any norm (the norm constraint makes impossible to multiply by constants other than ± 1), we consider V as a *metric* space, endowed with the distance d_G induced by $\|\cdot\|_{L^2(\Omega;\mathbb{R}^3)}$, i.e.

$$d_G((\mathbf{p},\mathbf{n}),(\mathbf{q},\mathbf{m})) := \|\mathbf{p}-\mathbf{q}\|_{L^2(\Omega;\mathbb{R}^3)} + \|\mathbf{n}-\mathbf{m}\|_{L^2(\Omega;\mathbb{R}^3)}, \tag{36}$$

and use Ambrosio, Gigli and Savaré's theory of gradient flows in metric spaces. In particular, we show that [2, Theorem 2.3.1], which deals with the existence of curves of maximal slope in metric spaces, can be applied to our problem.

We introduce below some of the relevant definitions, and refer the reader to [2] for complete details, and proofs.

The essential ingredients in the theory for metric spaces presented in [2] are a complete metric space $(\mathcal{S}, d)$, a functional $\phi\colon \mathcal{S} \to (-\infty, +\infty]$, with proper effective domain

$$D(\phi)\colon = \{v \in \mathcal{S} : \phi(v) < +\infty\} \neq \emptyset\},$$

and a (possibly) weaker topology σ on $\mathcal{S}$. The topology σ is also assumed to be a Hausdorff topology compatible with d, that is σ is weaker than the topology induced by d, and d is sequentially σ-lower semicontinuous, i.e.

$$(u_k, v_k) \overset{\sigma}{\to} (u, v) \Longrightarrow d(u, v) \leq \liminf_{k\to+\infty} d(u_k, v_k).$$

We define the *relaxed slope*, $|\partial^-\phi|$, of ϕ (see [2, (2.3.1)]) as

$$|\partial^-\phi|(v) := \inf\left\{\liminf_{k\to+\infty} |\partial\phi(v_k)| : v_k \overset{\sigma}{\to} v,\ \sup_k\{d(v_k, v), \phi(v_n)\} < +\infty\right\},$$

where $|\partial\phi|(v)$ is the *local slope* (see [2, Definition 1.2.4]):

$$|\partial\phi|(v) := \limsup_{w\to v} \frac{\max\{\phi(v) - \phi(w), 0\}}{d(w, v)}.$$

Note that if ϕ is smooth, one has $|\partial\phi|(v) = |\partial^-\phi|(v)$, and if in addition ϕ is Frechet differentiable, $|\partial^-\phi|$ is actually a strong upper gradient (see [2, Definition 1.2.1]) for ϕ, that is for every absolutely continuous curve $v : [a, b] \longrightarrow \mathcal{S}$ the function $|\partial^-\phi| \circ v$ is Borel, and it holds

$$|\phi(v(t)) - \phi(v(s))| \leq \int_s^t |\partial^-\phi|(v(r))|v_t(r)|\,dr \quad \text{for any } a < s \leq t < b,$$

with $|v_t|$ denoting the metric speed (see [2, (1.1.3)]):

$$|v_t(r)| := \lim_{s\to r} \frac{d(v(s), v(r))}{|s - r|}.$$

Finally, we say that a locally absolutely continuous map $u\colon (a, b) \to \mathcal{S}$ is a *curve of maximal slope* (see [2, Definition 1.3.2]), for the functional ϕ with respect to its upper gradient g, if $\phi \circ u$ is $\mathcal{L}^1$-*a.e.* equal to a non-increasing map φ, and

$$\varphi_t(r) \leq -\frac{1}{2}|u_t(r)|^2 - \frac{1}{2}g^2(u(r)) \quad \mathcal{L}^1\text{-}a.e. \text{ in } (a, b).$$

As per [2, Remark 1.3.3], if g is a strong upper gradient g, then $\phi(u(r)) \equiv \varphi(r)$ is a locally absolutely continuous map in (a, b), and the energy identity

$$\frac{1}{2}\int_s^t |u_t(r)|^2\,dr + \frac{1}{2}\int_s^t g^2(u(r))\,dr = \phi(u(s)) - \phi(u(t))$$

holds in each interval $[s, t] \subset (a, b)$.

In here, we pick

(i) $\mathcal{S} = V \cap \{G \leq G(\mathbf{p}_0, \mathbf{n}_0) + 1\}$ (with $(\mathbf{p}_0, \mathbf{n}_0)$ denoting the initial datum);

(ii) $d = d_G$;

(iii) $\phi = G$;

(iv) σ = topology induced on V by the weak topology of $L^2(\Omega;\mathbb{R}^3) \times L^2(\Omega;\mathbb{R}^3)$. As required, this is a Hausdorff topology on V compatible with d_G.

Completeness with respect to the distance d_G is proven in the following lemma.

Lemma 6.1. *For any $c > 0$, the metric space $(V \cap \{G \leq c\}, d_G)$ is complete.*

Proof. Consider an arbitrary Cauchy sequence $(\mathbf{p}_k, \mathbf{n}_k)_k \subseteq V \cap \{G \leq c\}$, since $\big(W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3), \|\cdot\|_{W^{1,2}\times W^{1,2}}\big)$ is a complete metric space, there exists $(\mathbf{p}, \mathbf{n}) \in W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3)$ such that $\mathbf{p}_k \to \mathbf{p}$, $\mathbf{n}_k \to \mathbf{n}$ in $W^{1,2}(\Omega;\mathbb{R}^3)$. By Sobolev embedding we have convergence a.e., hence from $(\mathbf{p}_k, \mathbf{n}_k) \in V$ we derive

$$|\mathbf{p}_k| \equiv |\mathbf{n}_k| \equiv 1 \Longrightarrow |\mathbf{p}| = |\mathbf{n}| = 1,$$
$$\mathbf{p}_k \cdot \mathbf{n}_k \equiv 0 \Longrightarrow \mathbf{p} \cdot \mathbf{n} = 0,$$

while the boundary conditions

$$\mathbf{p}_k(0) \equiv \mathbf{p}_k(1) \equiv (0,-1,0) \Longrightarrow \mathbf{p}(0) = \mathbf{p}(1) = (0,-1,0),$$
$$\mathbf{n}_k(0) \equiv \mathbf{n}_k(1) \equiv (\sin\theta_B, 0, \cos\theta_B) \Longrightarrow \mathbf{n}(0) = \mathbf{n}(1) = (\sin\theta_B, 0, \cos\theta_B).$$

follow from the trace theorem. In other words, we have $(\mathbf{p}, \mathbf{n}) \in V$. To prove that $(\mathbf{p}, \mathbf{n}) \in \{G \leq c\}$ we note that G is a sum of the convex function $\int_\Omega (|\nabla \mathbf{p}|^2 + |\nabla \mathbf{n}|^2 + 2\,p_1^2 + p_3^2)\,dx$ plus the linear function $\int_\Omega 2(1-p_2)\,dx$, and since convex (respectively, linear) functions are weakly lower-semicontinuous (respectively, continuous), we infer $G(\mathbf{p}, \mathbf{n}) \leq c$.

□

To apply [2, Theorem 2.3.1] to our problem, we also need to check some topological assumptions, which are included in Lemma 6.2 below.

Lemma 6.2. *The functional G satisfies the following properties:*

(A1) σ-lower semicontinuity: for any sequence $(\mathbf{p}_k, \mathbf{n}_k) \subseteq V$ σ-converging to some $(\mathbf{p}, \mathbf{n}) \in V$ we have

$$G(\mathbf{p}, \mathbf{n}) \leq \liminf_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k).$$

(A2) Coercivity: $G \geq 0$ in V.

(A3) Compactness: given a sequence $(\mathbf{p}_k, \mathbf{n}_k)_k \subseteq V$ with

$$\sup_k G(\mathbf{p}_k, \mathbf{n}_k) < +\infty, \qquad \sup_{k,h} d((\mathbf{p}_k, \mathbf{n}_k), (\mathbf{p}_h, \mathbf{n}_h)) < +\infty,$$

then we can extract a σ-converging sequence $(\mathbf{p}_{k_j}, \mathbf{n}_{k_j})_j$.

Proof. To show σ-lower semicontinuity, given a sequence $(\mathbf{p}_k, \mathbf{n}_k)_k$ σ-converging to $(\mathbf{p}, \mathbf{n})$, we need to check that

$$\liminf_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k) \geq G(\mathbf{p}, \mathbf{n}).$$

If $\liminf_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k) = +\infty$ then the thesis is trivial. Hence, without loss of generality we may assume

$$\liminf_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k) = \lim_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k) < +\infty,$$

and find N such that for all $k > N$ it holds $G(\mathbf{p}_k, \mathbf{n}_k) \leq C < +\infty$. In particular, since

$$G(\mathbf{p}_k, \mathbf{n}_k) \geq (\|\nabla \mathbf{p}\|^2_{L^2(\Omega;\mathbb{R}^3)} + \|\nabla \mathbf{n}\|^2_{L^2(\Omega;\mathbb{R}^3)}),$$

we have, upon removing the first N terms of the sequence,

$$\sup_k \left\{ \|\mathbf{p}\|^2_{W^{1,2}(\Omega;\mathbb{R}^3)} + \|\mathbf{n}\|^2_{W^{1,2}(\Omega;\mathbb{R}^3)} \right\} \leq C_1 < +\infty,$$

which implies that there exists $(\mathbf{p}', \mathbf{n}')$ such that $(\mathbf{p}_k, \mathbf{n}_k)$ converges to $(\mathbf{p}', \mathbf{n}')$ in the weak topology of $W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3)$. Next, again using the fact that convex (respectively, linear) functions are weakly lower semicontinuous (respectively, continuous), we infer as done at the end of the previous lemma that

$$G(\mathbf{p}', \mathbf{n}') \leq \liminf_{k\to+\infty} G(\mathbf{p}_k, \mathbf{n}_k).$$

Finally, remembering that $(\mathbf{p}_k, \mathbf{n}_k)_k$ σ-converges to $(\mathbf{p}, \mathbf{n})$, we obtain $(\mathbf{p}, \mathbf{n}) = (\mathbf{p}', \mathbf{n}')$, and G is σ-lower semicontinuous.

The coercivity condition (A2) follows from the definition of G.

To prove the compactness (A3), we use the fact that $\sup_k G(\mathbf{p}_k, \mathbf{n}_k) < +\infty$ and

$$G(\mathbf{p}_k, \mathbf{n}_k) \geq (\|\nabla \mathbf{p}_k\|^2_{L^2(\Omega;\mathbb{R}^3)} + \|\nabla \mathbf{n}_k\|^2_{L^2(\Omega;\mathbb{R}^3)}),$$

give $(\mathbf{p}_k, \mathbf{n}_k)_k$ uniformly bounded in $W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3)$, which implies that (up to subsequences) there exists $(\mathbf{p}, \mathbf{n}) \in W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3)$ such that $\mathbf{p}_k \to \mathbf{p}$, $\mathbf{n}_k \to \mathbf{n}$ weakly in $W^{1,2}(\Omega;\mathbb{R}^3) \times W^{1,2}(\Omega;\mathbb{R}^3)$, strongly in $L^2(\Omega'\mathbb{R}^3) \times L^2(\Omega'\mathbb{R}^3)$, and a.e. in Ω. We conclude $(\mathbf{p}, \mathbf{n}) \in V$ and $G(\mathbf{p}, \mathbf{n}) < \sup_k G(\mathbf{p}_k, \mathbf{n}_k)$, as in Lemma 6.1. ☐

Theorem 6.3. *For any $T > 0$ and initial datum $(\mathbf{p}_0, \mathbf{n}_0) \in V$, there exists a curve*

$$(\mathbf{p}(t), \mathbf{n}(t)) : [0, T] \longrightarrow V, \qquad (\mathbf{p}(0), \mathbf{n}(0)) = (\mathbf{p}_0, \mathbf{n}_0)$$

of maximal slope solution of $|u_t(t)| = -|\partial G|(t)$ for a.e. $t \in [0, T]$.

Proof. Thanks to Lemmas 6.1 and 6.2, we are able to apply Theorem 2.3.1 in [2] with $\mathcal{S} = V \cap \{G \leq G(\mathbf{p}_0, \mathbf{n}_0)+1\}$, $\phi = G$, $d = d_G$ and σ the topology induced on V by the weak topology of $L^2(\Omega;\mathbb{R}^3)\times L^2(\Omega;\mathbb{R}^3)$. Additionally, since G is smooth and Frechet differentiable, we have that $|\partial^- G| = |\partial G|$, and $|\partial G|$ is a strong upper gradient. Therefore, we can conclude that every curve $(\mathbf{p}(t), \mathbf{n}(t)) \in GMM((\mathbf{p}_0, \mathbf{n}_0))$ is a curve of maximal slope for G with respect to $|\partial G|$, and that the following energy identity holds

$$\frac{1}{2}\int_0^T |(\mathbf{p}_t(r), \mathbf{n}_t(r))|^2\, dr + \frac{1}{2}\int_0^T |\partial G|^2(\mathbf{p}(r), \mathbf{n}(r))\, dr = G(\mathbf{p}_0, \mathbf{n}_0) - G(\mathbf{p}(T), \mathbf{n}(T)).$$

Here $GMM((\mathbf{p}_0, \mathbf{n}_0))$ denotes the set of generalized minimizing movements (see [2, Definition 2.0.6]) of G starting at the initial datum $(\mathbf{p}_0, \mathbf{n}_0) \in V$.

Our theorem is then proven by noticing that [2, Proposition 2.2.3] implies that the set $GMM((\mathbf{p}_0, \mathbf{n}_0))$ is non-empty. □

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